Direct Numerical Simulation of Polycrystal

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We performed several direct numerical simulations to investigate the polycrystal behavior in certain metals when subjected to strong shocks. Figure 1 shows the initial configuration and a shock generated by PBX 9501 at Chapman-Jouguet (C-J) pressure on the left side of the structure passing through a 50 × 50 μm metal plate composed of two distinct phases of different densities and compressibilities. Each element of 100 × 100 × 1 hexahedral grid was subdivided into four prisms to generate a triangular grid of 40000 prismatic elements to resolve interfaces between the two phases. It is not possible to complete this calculation in a Lagrangian mode because of the amount of turbulence generated at later times. Thus the calculation was carried out by moving the entire mesh "window" with the average fluid velocity of the domain. The CHAD code [1, 2] with the interface tracking/reconstruction capability turned off was employed for this calculation. The left boundary was modeled by a constant-velocity piston until the shock cleared the plate, and then it was changed into an inflow-outflow pressure-specified boundary. The right boundary was treated as inflow/outflow pressure-specified boundary throughout the transient. The bottom and top boundaries were reflective.

Figure 2 shows the comparison of initial density and density at 1000 ns, about 990 ns after the shock has passed the plate. A considerable distortion and mixing are observed at this time. A clear evidence of mixing and turbulence is shown by the vorticity contours of Fig. 3.

Figure 4 shows the fluctuating component of x-direction velocity $\overline{u'u'}$ and its normalized value as a function of time. The exact expressions of how the fluctuation component is defined also are given in Fig. 4. These values are averages over the entire domain and not over any cross section. The cross-sectional values are not meaningful because a meaningful estimate would require numerous calculations with different polycrystal sizes and orientations. By the same argument the data in Fig. 4 are also not meaningful before ~20 ns because it took ~10 ns for the shock to pass through the calculational domain. A significant finding of this calculation is the surprising amount of ~15% kinetic energy in the turbulence field near 100 ns. Such strong turbulence could have significant implications for integral system calculations.

We plan to perform a macrocalculation using a statistically similar sample of several mm size under similar hydrodynamics conditions using the BHR turbulence model [3]. It will be interesting to find out if such a model could predict a similar amount of turbulence kinetic energy.

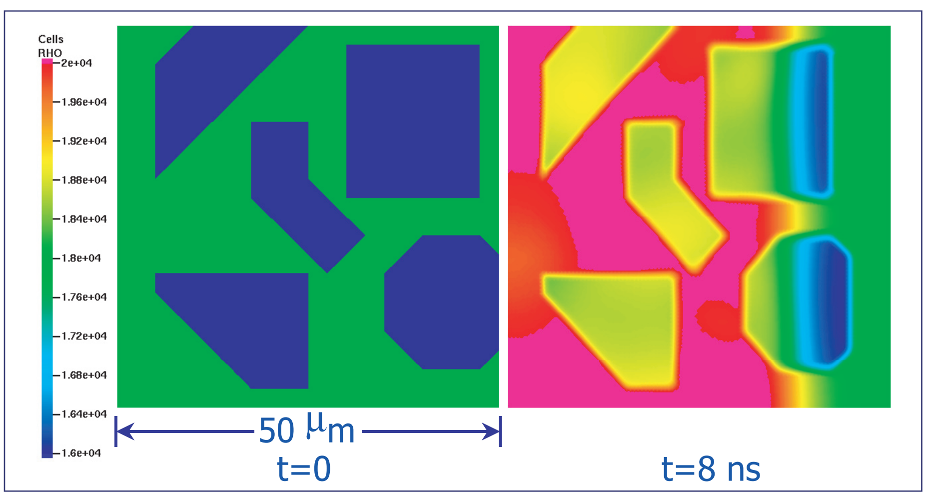

Figure 1— ***Initial shock propagation of a strong shock through the two phases of a polycrystal structure. The continuous phase has higher density but lower sound speed.***

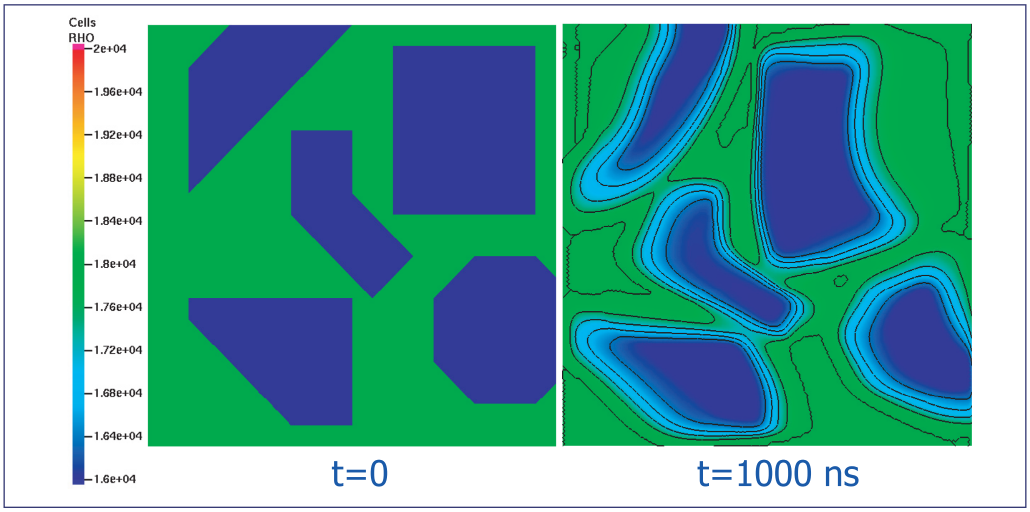

Figure 2— Comparison of the initial density contours with those at 1000 ns.

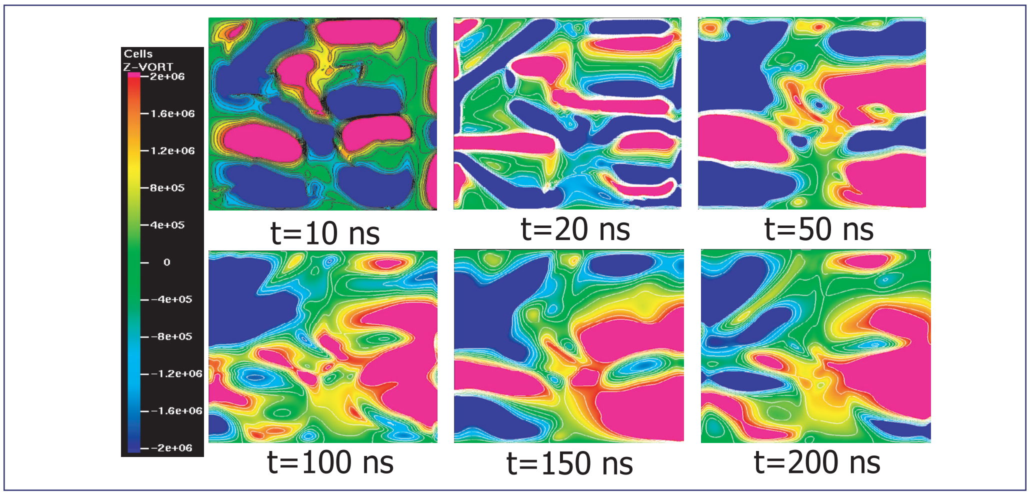

Figure 3— Snapshots of vorticity contours.

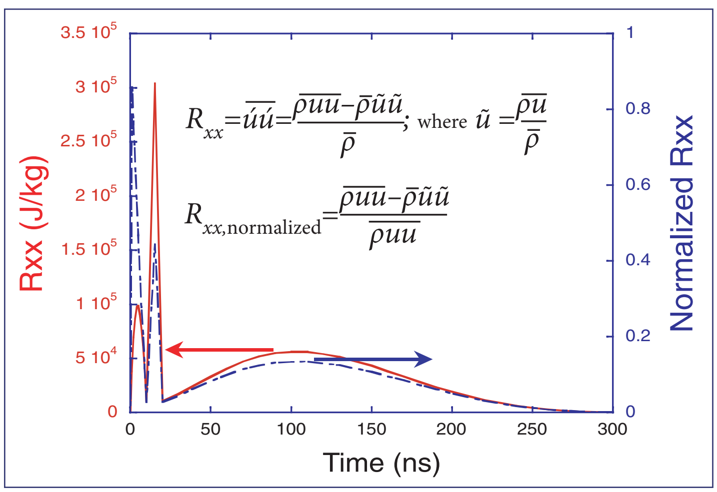

Figure 4— Turbulence kinetic energy history.

[1] P.J. O'Rourke and M.S. Sahota, "CHAD: A Parallel, 3-D, Implicit, Unstructured-Grid, Multimaterial, Hydrodynamics Code for all Flow Speeds, Los Alamos National Laboratory report, LA-UR-98-5663 (October 1998).

[2] P.J. O'Rourke and M.S. Sahota, *J. Comp. Phys.* **143** (1998), pp. 312–345.

[3] Didier Besnard, et al., "Turbulence Transport Equations for Variable-Density Turbulence and Their Relationship to Two-Field Models," Los Alamos National Laboratory report LA-12303-MS (June 1992).

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